McGill
Faculty of Engineering

Course Outline
CHEE440

Course Title: **Process Modeling**
Credits: **3**
Contact Hours: **(3-1-5)**
Course Prerequisite(s): **CHEE 423, MATH 264.**
Course Corequisite(s): **N/A**
Course Description: **Principles of mathematical modelling in chemical engineering: problem formulation, solution, discrete systems; difference and difference-differential equations, methods of solution; understanding system behaviour, optimization.**

Canadian Engineering Accreditation Board (CEAB) Curriculum Content

CEAB curriculum category content	Number of AU's	Description
Math	**22.8**	Mathematics include appropriate elements of linear algebra, differential and integral calculus, differential equations, probability, statistics, numerical analysis, and discrete mathematics.
Natural science	**0**	Natural science includes elements of physics and chemistry, as well as life sciences and earth sciences. The subjects are intended to impart an understanding of natural phenomena and relationships through the use of analytical and/or experimental techniques.
Complementary studies	**0**	Complementary studies include the following areas of study to complement the technical content of the curriculum: engineering economics; the impact of technology on society; subject matter that deals with central issues, methodologies, and thought processes of the arts, humanities and social sciences; management; oral and written communications; healthy and safety; professional ethics, equity and law; and sustainable development and environmental stewardship.
Engineering science	**22.8**	Engineering science involves the application of mathematics and natural science to practical problems. They may involve the development of mathematical or numerical techniques, modeling, simulation, and experimental procedures. Such subjects include, among others, applied aspects of strength of materials, fluid mechanics, thermodynamics, electrical and electronic circuits, soil mechanics, automatic control, aerodynamics, transport phenomena, elements of materials science, geoscience, computer science, and environmental science.
Engineering design	**0**	Engineering design integrates mathematics, natural sciences, engineering sciences, and complementary studies in order to develop elements, systems, and processes to meet specific needs. It is a creative, iterative, and open-ended process, subject to constraints which may be governed by standards or legislation to varying degrees depending upon the discipline. These constraints may also relate to economic, health, safety, environmental, societal or other interdisciplinary factors.

Accreditation units (AU's) are defined on an hourly basis for an activity which is granted academic credit and for which the associated number of hours corresponds to the actual contact time: one hour of lecture (corresponding to 50 minutes of activity) = 1 AU; one hour of laboratory or scheduled tutorial = 0.5 AU. Classes of other than the nominal 50-minute duration are treated proportionally. In assessing thetime assigned to determine the AU's of various components of the curriculum, the actual instruction time exclusive of final examinations is used.

Graduate Attributes

This course contributes to the acquisition of graduate attributes as follows:

Graduate attribute	KB	PA	IN	DE	ET	IT	CS	PR	IE	EE	EP	LL
Level descriptor	A	A	I	N/A	N/A	N/A	N/A	N/A	NA	N/A	N/A	N/A

n/a = Not applicable; I = Introduced; D = Developed; A = Applied

KB *- Knowledge Base for Engineering: Demonstrated competence in university level mathematics, natural sciences, engineeringfundamentals, and specialized engineering knowledge appropriate to the program.*

PA *- Problem Analysis: An ability to use appropriate knowledge and skills to identify, formulate, analyze, and solve complex engineeringproblems in order to reach substantiated conclusions.*

IN *- Investigation: An ability to conduct investigations of complex problems by methods that include appropriate experiments, analysis andinterpretation of data, and synthesis of information in order to reach valid conclusions.*

DE *- Design: An ability to design solutions for complex, open-ended engineering problems and to design systems, components or processesthat meet specified needs with appropriate attention to health and safety risks, applicable standards, economic, environmental, cultural and societal considerations.*

ET *- Use of Engineering Tools: An ability to create, select, adapt, and extend appropriate techniques, resources, and modern engineeringtools to a range of engineering activities, from simple to complex, with an understanding of the associated limitations.*

IT *- Individual and Team Work: An ability to work effectively as a member and leader in teams, preferably in a multi-disciplinary setting.*

CS *- Communication Skills: An ability to communicate complex engineering concepts within the profession and with society at large. Suchabilities include reading, writing, speaking and listening, and the ability to comprehend and write effective reports and design documentation, and to give and effectively respond to clear instructions.*

PR *- Professionalism: An understanding of the roles and responsibilities of the professional engineer in society, especially the primary roleof protection of the public and the public interest.*

IE *- Impact of Engineering on Society and the Environment: An ability to analyse social and environmental aspects of engineering activities.Such abilities include an understanding of the interactions that engineering has with the economic, social, health, safety, legal, and cultural aspects of society; the uncertainties in the prediction of such interactions; and the concepts of sustainable design and development and environmental stewardship.*

EE *- Ethics and Equity: An ability to apply professional ethics, accountability, and equity.*

EP *- Economics and Project Management: An ability to appropriately incorporate economics and business practices including project, riskand change management into the practice of engineering, and to understand their limitations.*

LL *- Life-Long Learning: An ability to identify and to address their own educational needs in a changing world, sufficiently to maintain theircompetence and contribute to the advancement of knowledge.*

Policies

Academic Integrity

McGill University values academic integrity. Therefore, all students must understand the meaning and consequences of cheating, plagiarism and other academic offences under the Code of Student Conduct and Disciplinary Procedures. (see www.mcgill.ca/students/srr/honest/ for more information). (approved by Senate on 29 January 2003)

In accord with McGill University's Charter of Students' Rights, students in this course have the right to submit in English or in French any written work that is to be graded.

(approved by Senate on 21 January 2009)

Grading Policy

In the Faculty of Engineering, letter grades are assigned according to the grading scheme adopted by the professor in charge of a particular course. This may not correspond to practices in other Faculty and Schools in the University.

In the event of extraordinary circumstances beyond the University's control, the content and/or evaluation scheme in this course is subject to change.

McGill

Faculty of Engineering

CHEE 440 Process Modeling

Winter 2016

CLASS SCHEDULE

Lectures : MW 2:35-3:55, Wong Bldg. 1020, Jan 07 – Apr 15.

INSTRUCTOR

Alejandro D. Rey, James McGill Professor
Office: Wong 4100
Phone: 398-4196
Email: alejandro.rey@mcgill.ca

Office hours: M 16:00-17:00

TUTORIALS

F 4:35-5:25, Trottier 0100, Jan 07 – Apr 15

TEACHING ASSISTANTS (TAS)

Mohammadamin Sadeghi Mohammadamin Sadeghi

Oscar Matus Rivas oscar.matusrivas@mail.mcgill.ca

Zeina Jendi zeina.jendi@mail.mcgill.ca

Teaching assistants will provide limited assistance with course material during the tutorials and will be responsible for assignments and quizzes.

COMMUNICATION

My personal website (accessible via http://rey1.chemeng.mcgill.ca/)and myCourses will be used to distribute course information. If you need to reach me, please send an email to alejandro.rey@mcgill.ca. I will try to respond within 48 hours. If you have questions about the material please come to my designated office hours or schedule an appointment. Specific questions about problems or theory will not be answered through email. If you have questions about the assignments please see the assigned teaching assistant at his/her designated office hours or schedule an appointment.

Class Participation

Students must pre-read the assigned material and are expected to participate in the class lectures. Mobile devices are not allowed at any time. Students disturbing the learning and teaching process will be asked to leave the classroom.

COURSE MATERIALS

- CLASS NOTES: "Process Modeling" (Available at Copy-EUS McConnell Eng Bldg)
- Scientific pocket calculator. Only an official Faculty of Engineering approved standard calculator may be used during examinations
  http://www.mcgill.ca/engineering/student/sao/policies/examinations/calculators/
- Lecture notes and slides. Instructor generated course materials (e.g., handouts, notes, summaries, exam questions, etc.) are protected by law and may not be copied or distributed in any form or in any medium without explicit permission of the instructor. Note that infringements of copyright can be subject to follow up by the University under the Code of Student Conduct and Disciplinary Procedures. All quizzes and midterm examination materials must be returned after the examinations.

LEARNINGOBJECTIVES

1. Develop working knowledge of the science of mathematical modeling in chemical engineering process.
2. Develop system-based analytical skills to integrate chemical engineering processes and process modeling.
3. Develop the mathematical skills to solve process models for design, control and prediction.

INSTRUCTIONAL METHODS

The course will involve lectures, tutorials and office hours. The students are required to pre-read the assigned class notes before attending each class. Weekly class lectures cover course material not found in the class notes.

MISSED ASSIGNMENT ,QUIZ AND EXAM POLICIES

The weight of a missed assignment, quiz and/or midterm exam will be carried automatically to the final exam.

POLICY FOR QUIZ AND EXAM REVIEWS

Quizzes: This will be done individually in the TA's office only during office hours and no later than two weeks after you are informed of your grade (For other times please request your appointments by email). Midterm: This will be done individually in the TA's office (Quizz 1: Jendi and Quiz 2: Matus Rivas) only during office hours and no later than two weeks after you are informed of your grade (For other times please request your appointments by email). After that, no request will be granted. Failing this, you will be asked to make an official request with the Student Affairs office.

EVALUATION AND ASSESSMENT

The students will be responsible for submitting the assignments at the beginning of each tutorial. Late submissions will be returned ungraded. There will be 10 assignments, 2 quizzes, 1 midterm examination and 1 final exam. All weight of missed assignments, quizzes and examination will be carried to the final exam for the course. Under no circumstances will there be make up assignments, quizzes, midterm and/or final exams.

ASSIGNMENTS (A1-A10)

The assignments are individual work. If pictures and graphs are taken from websites and copyrighted texts, proper referencing must be done. Be thorough and clear. The ten assignments are found at the back of the class notes.

QUIZZES AND EXAMINATION RULES

The 50 minutes quizzes, 60 minutes midterm exam and 3 hours final exam are closed books, closed notes, and closed electronic devices. For Quiz 1 and 2, bring ONE single sided 8 1/2 by 11 formula sheet. For the midterm bring a double sided 81/2 by 11 formula sheet. For the final bring 2 double sided 81/2 by 11 formula sheets. Only the faculty calculator is allowed. All other material and devices are not allowed .

Quiz contents:
Quiz #1: Lectures 1-11 (Matus Rivas)
Quizz #2: Lectures 12-23 (Jendi)
Midterm contents:
Lectures 1-16 (Prof. Rey)
The final exam is all inclusive. The 50 minute quizzes will take place during the tutorial hour. The location of the midterm (March 9 at 2:35-3:45 PM) is :

A-H: Wong Bldg, Room 1020 (Sadeghi)
I-Z: Macdonald Eng. Bldg., Room 280 (Jendi and Matus Rivas)

MARK DISTRIBUTION

10 Assignments	5%	*Friday, Jan 15,22,29; Feb 5,19,26; March 11,18, April: 1, 15.*
2 Quizzes (50 min each)	20%	*Friday, Feb 12 (Matus Rivas); April 1 (Jendi).*
Midterm examination (60 min)	25%	*Wednesday, March 9 (Prof. Rey).*
Final examination (3 hours)	50%	*TBA (Prof. Rey).*

NB: THE SCHEDULE MAY BE SUBJECTED TO CHANGE DURING THE SEMESTER.

Assignment Schedule and Responsible TA

Assignment #1, FRIDAY January 15: Sadeghi

Assignment #2, FRIDAY January 22: Sadeghi

Assignment #3, FRIDAY January 29: Matus Rivas

Assignment #4, FRIDAY February 11: Matus Rivas

Assignment #5, Wednesday February 18: Sadeghi

Study Break: March 2-6

Assignment #6 , Wednesday March 11: Jendi

Assignment #7, Wednesday March 18: Sadeghi

Assignment #8, Wednesday March 25:Jendi

Assignment #9, Wednesday April 8 : Matus Rivas

Assignment #10, Wednesday April 15: Jendi

SCHEDULE

THE SCHEDULE MAY BE SUBJECTED TO CHANGE DURING THE SEMESTER.

Week # Date Chapter	**Topic**	**PreRead (class notes)**	**Assignment Due (Fridays)**	**Quiz Date and #**
Week #0 9/9-9/11 Lecture 1	Syllabus Modelling Eng. Process	1.1 Appendix 2	-	-
Week #1 1/11,1/13 Lecture 2-3	Process Models Microscopic Models; Scaling; Dimensionless Numbers	1.2.1-1.2.2 1.2.3-1.2.7 Appendix 1,4	A1	Tutorial 1
Week #2 1/18,1/20 Lecture 4-5	Multiple Gradient; Models, Dispersion	1.2.2.3 Appendix 1,4,6	A2	Tutorial 2
Week #3 1/25,1/27 Lecture 6-7	Maximum Gradient; and Macroscopic Models	1.2.2.4-5	A3	Tutorial 3
Week #4 2/1,2/3 Lecture 8-9	Macroscopic and Mixed Models; Strategies; Examples.	1.2.2.5 1.3-1.4	A4	Tutorial 4
Week #5 2/8-2/10 Lecture 10-11	Model Response; Delta- impulse Func.; Frequency Response; Transfer Function; Residence Time.	1.5	NO assignment	**Quiz #1 (50min) Feb 12**

Week #6 2/15-2/17 Lecture 12-13	Model Response ; PDE's.	1.5 2.1.1-2 Appendix 3 Appendix 5	A5	Tutorial 5
Week #7 2/22-2/24 Lecture 14-15	Similarity; Sources; Images; Superposition.	2.1.2	A6	Tutorial 6
Week #8 3/7-**3/9 (Midterm)** Lecture 16	Similarity; Sources; Images; Superposition.	2.1.2	A7	Tutorial 7
Week #9 3/14-3/16 Lecture 17-18	Hyperbolic PDEs; Method of Characteristics.	2.1.3 Appendix 7	A8	Tutorial 8
Week #10 3/21-3/23 Lecture 19-20	Method of Characteristics; Separations of Variables.	2.1.3; 2.1-4 Appendix 5, 7	Easter	Easter Friday
Week #11 3/30 Lecture 20 Easter Monday	Discrete Models	2.2 .1-3 2.3	No assignment	**Quiz #2 (50 min) April 1**
Week #12 4/4-4/6 Lecture 22-23	Discrete Models	2.3	A9	Tutorial 9
Week #13 4/11-4/13 Lecture 24-25	Discrete Models,; Summary	2.3	A10	Tutorial 10

LIST OF TOPICS

4 Sections and 26 Topics

A. Continuous Models in Chemical Engineering

(i) Basic Modelling Elements

1. Vectors, coordinate systems, ODEs (Laplace transforms, systems ODEs), multivariable calculus.
2. Control volume (stationary, moving, deforming) and fundamental balance equation.
3. Eulerian and Lagrangean coordinates
4. Divergence theorem, Leibnitz theorem, Reynolds theorem, material derivative, integral theorems
5. Constitutive equations and fluxes
6. Processes: convection, diffusion, laminar and turbulent dispersion, reaction, sedimentation, adsorption, absorption, agglomeration, phase transitions.

(ii)Derivation of Main Models and their Applications

7. Models: microscopic, multiple gradient, maximum gradient, mixed models (micro-macro, porous media, plug flow with axial dispersion)

(iii) Particular Solutions

8. Boundary and initial conditions, classification (Dirichlet, Neumann, Robin)

(iv) Approximations and Simplifications

9. Dimensionless numbers, scaling, order of magnitude.

(v) Control, Design and Prediction

10. Response methods: pulse, step, frequency response(Bode plots) for single and multiple reactors, mixers, and heaters, residence time distributions

B. Partial Differential Equations in Chemical Engineering: Solution Methods and Applications

(vi) PDE's in Chemical Engineering

11. Classification and examples: elliptic, parabolic, hyperbolic

(vii) Integration of PDE's Solution Methods, Models, and Processes in Chemical Engineering

12. Integral method
13. Similarity solutions
14. Method of sources
15. Superposition of sources in time and space
16. Method of images
17. Method of characteristics
18. Separation of variables

C. Discrete Models in Chemical Engineering

(viii) Discrete Processes in Chemical Engineering

19. Stage operations, reactor batteries.

(ix) Discrete Mathematics

20. Discrete calculusoperators
21. Newton's forward difference
22. Applications to interpolation and extrapolation of experimental data
23.Linear, nonlinear (Riccati), coupled difference equations

D. Applications of Discrete Models to Chemical Engineering

24. Discretization of continuous models
25. Staged operations
26. Optimization, Lagrange multipliers

DETAILEDCOURSECONTENTS2016

PART I : Principles of Process Modelling

I.1 Modelling Process

I.1.1 Introduction

I.1.2 Three Methodologies

I.1.2.1 Fundamental Method

I.1.2.2 Empirical Method

I.1.2.3 Analogy

- I.1.3 Why Model ?
- I.1.4 Role of Objectives
- I.1.5 Constructing a Model
  - I.1.5.1 Elements and Procedure
  - I.1.5.2 Conservation Laws
  - I.1.5.3 Constitutive Equations
- I.1.6 Modelling Logic

I.2 Formulation of Mathematical Problem

- I.2.1 Vector Analysis
- I.2.2 Types of Models
  - I.2.2.1 General Categorisation
  - I.2.2.2 Microscopic Balances
  - I.2.2.3 Multiple Gradient Models
  - I.2.2.4 Maximum Gradient Models
  - I.2.2.5 Macroscopic Balances
- I.2.3 Equations of State
- I.2.4 Chemical and Phase Equilibrium
- I.2.5 Rate Equations
- I.2.6 Integral Representation of Models
- I.2.7 Boundary and Initial Conditions

I.3 Solution method strategies:

- I.3.1 Introduction
- I.3.2 Exact Models
- I.3.3 Simplifying Assumptions and Approximate Models
- I.3.4 Exact Solutions to Approximate Equations
- I.3.5 Solution Consistency

I.4 Classification of Mathematical Models

- I.4.1 Distributed versus Lumped Parameter Models